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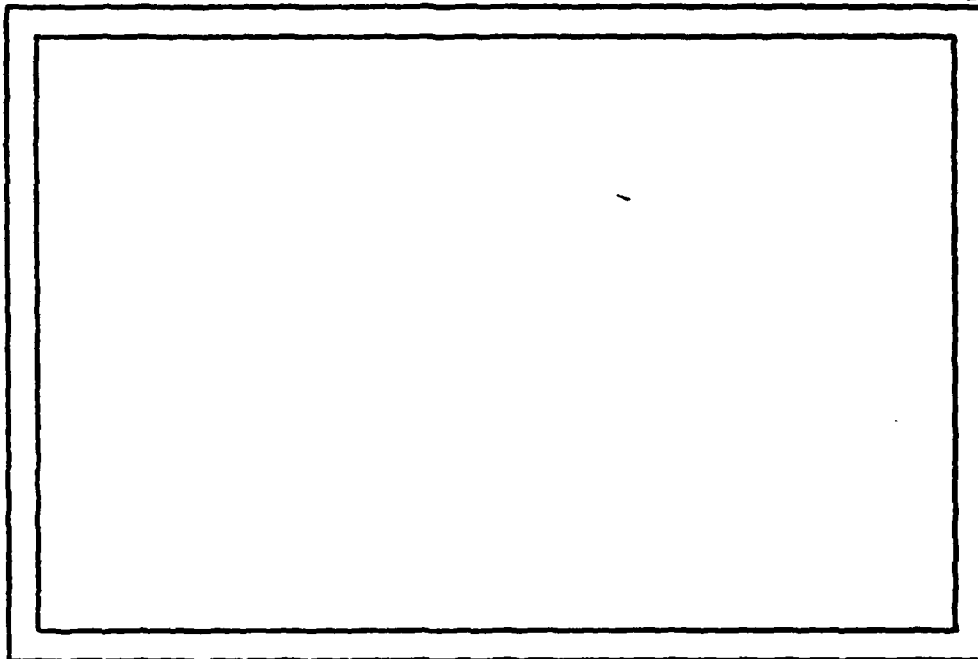
The figure is a Total Ion Chromatogram (TIC) plot. The y-axis is labeled 'Abundance' and ranges from 0 to 1,000,000. The x-axis is labeled 'Time (min)' and ranges from 0 to 20. A single, very sharp and intense peak is visible at approximately 10.5 minutes, reaching an abundance of nearly 1,000,000. The baseline is flat and stable at approximately 100,000 abundance units throughout the rest of the run.

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ON AN ESTIMATION SCHEME FOR  
GAUSS MARKOV RANDOM FIELD MODELS

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ABSTRACT

In an earlier report [1] a consistent estimation scheme was given for Gaussian Markov random field models. In this report we consider some statistical properties of the resulting estimate. Specifically, we derive an expression for the asymptotic mean square error of the estimate for a general model and compare the efficiency of this estimate with the popular coding estimate for a simple first order isotropic model.

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## 1. Introduction

Markov random field (MRF) models are of much interest in image analysis and processing. For instance, they have been used in texture analysis [2,3] and image restoration [4-6]. They are also of interest in the analysis of field data [7]. MRF models characterize the special nature of the statistical dependency of intensity levels over a neighborhood in an image. If  $y(s)$  denotes the intensity level at location  $s$ , then  $y(s)$  is written as a linear combination of intensity levels  $\{y(s+r)$ ,  $r \in N\}$  (where  $N$  is known as the neighbor set of dependence) and additive noise. The members of set  $N$  are pairs of integers  $(k,l)$  not including  $(0,0)$ . For example, the first order MRF model results when  $N = \{(0,1), (1,0), (0,-1), (-1,0)\}$  and the second order MRF model results when  $N = \{(-1,0), (1,0), (0,-1), (0,1), (-1,-1), (-1,1), (1,-1), (1,1)\}$ . Each MRF model is characterized by a set of linear weights and the variance of the additive noise.

Suppose we are given an array of intensity level variations  $\{y(s), s \in \Omega\}$ ,  $\Omega = \{s: (i,j), 1 \leq i,j \leq M\}$  and we are interested in fitting a Gaussian MRF model to this data. We also assume that the specific structure of the MRF model characterized by the neighbor set  $N$  is known. The problem of estimating  $N$  has been considered elsewhere [1,8]. Three estimation methods, namely the coding method [7], the maximum likelihood (ML) method, and the method in [9] can be used to obtain estimates of parameters characterizing a MRF model. It is the intent of this paper to analyze in some detail the statistical properties of the estimate in [1,8].

Specifically, we shall derive an expression for the asymptotic mean square error of the estimate for an arbitrary MRF model. We evaluate this expression for a simple first order isotropic MRF model and compare the efficiency of the estimate with the popular coding estimate.

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## 2. Estimates and their statistical properties in MRF models

### 2.1 Model Representation

Assume that the given image data  $\{y(s)\}$  obeys the MRF model in (2.1), with the associated neighbor set  $N$ :

$$y(s) = \sum_{r \in N} \theta_r y(s+r) + e(s), s \in \Omega, \quad (2.1)$$

In (2.1) the neighbor set  $N$  is symmetric, i.e., if  $r \in N$  then  $-r \in N$ . Further, the coefficients satisfy the constraint  $\theta_r = \theta_{-r}$ . The stationary noise sequence  $\{e(s)\}$  is partly characterized by

$$E(e(s) | y(r)) = 0 \quad \forall s \neq r \quad (2.2)$$

Using (2.1) and (2.2) one can prove that the noise sequence  $\{e(s)\}$  is correlated with the correlation structure

$$\begin{aligned} E(e(s) e(r)) &= v, & s=r \\ &= -\theta_{s-r} v, & (s-r) \in N \\ &= 0 & \text{otherwise} \end{aligned} \quad (2.3)$$

It can be shown by methods similar to [10,11] that an observation  $y(s)$  obeying (2.1) with the conditions (2.3) indeed satisfies the Markov condition

$$\begin{aligned} p(y(s) | y(r), r \in \Omega, r \neq s) \\ = p(y(s) | y(s+t), t \in N) \end{aligned}$$

We shall characterize the neighbor set for the MRF model using the set  $N_S$ , which includes members from the non-symmetric half of  $N$ , i.e., if  $s \in N_S$  then  $-s \in N_S$  and  $N = \{s: s \in N_S\} \cup \{-s: s \in N_S\}$ . A sufficient condition to ensure stationarity is [7]

$$\sum \sum \theta_{k,l} z_1^k z_2^l < 1 \text{ whenever } |z_1| = |z_2| = 1$$

## 2.2 A consistent estimation scheme [1, 8]:

Consider the estimates

$$\hat{\theta}^* = \left[ \sum_{\Omega_I} \underline{q}(s) \underline{q}^T(s) \right]^{-1} \left( \sum_{\Omega_I} \underline{q}(s) y(s) \right) \quad (2.4)$$

and

$$v^* = \frac{1}{M^2} \sum_{\Omega_I} (y(s) - \hat{\theta}^{*T} \underline{q}(s))^2 \quad (2.5)$$

where

$$\Omega_I = \Omega - \Omega_B$$

and

$$\Omega_B = \{s = (i, j) : s \in \Omega \text{ and } (s+r) \notin \Omega \text{ for at least one } r \in N\}$$

We now state a theorem regarding the consistency of the estimate  $\hat{\theta}^*$  and give an expression for the asymptotic variance of the estimate  $\hat{\theta}^*$ . An expression for the asymptotic variance of  $\hat{\theta}^*$  for an isotropic MRF model with  $N_S = \{(0,1), (1,0)\}$  is also given.

Theorem 1: Let  $y(s)$ ,  $s \in \Omega$  be the set of observations obeying the MRF model (2.1). Then

- (i) The estimate  $\hat{\theta}^*$  is asymptotically consistent.
- (ii) The asymptotic covariance matrix of  $\hat{\theta}^*$  is

$$\begin{aligned} E(\hat{\theta} - \hat{\theta}^*)(\hat{\theta} - \hat{\theta}^*)^T &= \frac{1}{M^2} [v \underline{Q}^{-1} + 2v^2 (\underline{Q}^T \underline{Q})^{-1} \\ &\quad - \frac{v}{M^2} \underline{Q}^{-1} \sum_{\substack{s, r \\ (s-r) \in N}} \sum \theta(s-r) \underline{T}_{r,s} (\underline{Q}^T)^{-1}] \end{aligned} \quad (2.6)$$

where

$$\underline{Q} = E[\underline{q}(s) \underline{q}^T(s)]$$

and

$$\underline{T}_{r,s} = E[\underline{q}(r) \underline{q}^T(s)]$$

(iii) For the isotropic conditional model with  $N_S = \{(0,1), (1,0)\}$ , the asymptotic expected mean square error is

$$E(\theta - \theta^*)^2 = \frac{2\theta^2(1-4\theta\alpha_{1,0})^2}{4M^2\alpha_{1,0}^2} \quad (2.7)$$

$$\alpha_{1,0} = \frac{\text{cov}(y(s), y(s+(1,0)))}{\text{cov}(y^2(s))} \quad (2.8)$$

The elements of matrices  $\underline{Q}$  and  $\underline{T}_{r,s}$  are functions of normalized autocorrelation coefficients  $\alpha_{k,l}$ . The proof is given in Appendix I.

Although  $\theta^*$  is a consistent estimate of  $\theta$ , it is not very efficient. We compare the efficiency of this estimate with efficiencies of the coding estimate for a simple MRF model with  $N_S = \{(0,1), (1,0)\}$ . The exact ML estimate is obtained by assuming a toroidal lattice representation for  $y(s)$  and maximizing the resulting log likelihood function by using the Newton-Raphson procedure. Equation (2.4) can also be used for toroidal lattice representation by summing over  $\Omega$  instead of  $\Omega_I$ . The resulting difference in the numerical value is negligible for sufficiently large  $M$ .



### 2.3 Comparison of estimates

We compare the asymptotic variance of the estimate (2.4) with the asymptotic variances of the coding estimate and ML estimate for the isotropic conditional models with  $N_S = \{(0,1), (1,0)\}$ . From [9], the asymptotic variance of the coding estimate  $\theta_C$  is

$$M^2 \text{Var}(\theta_C) = \frac{\theta(1-4\theta\alpha_{1,0})}{2\alpha_{1,0}} \quad (2.9)$$

Also from [9], the variance of the ML estimate  $\theta_{ML}$  is

$$\text{Var}(\theta_{ML}) = \frac{0.5}{M^2 (I(\theta) - 4V_{10}^2(\theta))} \quad (2.10)$$

where

$$I(\theta) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{(\cos x + \cos y)^2 dx dy}{(1-2\theta(\cos x + \cos y))^2}$$

and

$$V_{st}(\theta) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{\cos(sx+ty) dx dy}{(1-2\theta(\cos x + \cos y))}$$

Tabulated values of  $V_{10}(\theta)$ ,  $\alpha_{1,0}$  and  $I(\theta)$  are available in [9] for different values of  $\theta$ . Using these values, and (2.7), (2.9) and (2.10), columns 2-4 of Table I are computed. The asymptotic efficiencies in columns 5 and 6 are defined by

$$\text{eff}(\theta_C) = \frac{\text{Var}(\hat{\theta}_{ML})}{\text{Var}(\theta_C)}$$

and

$$\text{eff}(\theta^*) = \frac{\text{Var}(\hat{\theta}_{ML})}{\text{Var}(\theta^*)}$$

It is evident that the estimate  $\hat{\theta}^*$  computed using (2.4) is more efficient than the coding estimate but is not as good as the ML estimate. Note that column 5 is available in [9].

## Appendix I

proof of Theorem 1:

i) We have from (2.4)

$$\underline{\theta}^* = \left[ \sum_{\Omega_I} \underline{q}(s) \underline{q}^T(s) \right]^{-1} \left( \sum_{\Omega_I} \underline{q}(s) y(s) \right) \quad (1)$$

Substituting for  $y(s)$  from (2.1) and simplifying, we have

$$\left[ \sum_{\Omega_I} \underline{q}(s) \underline{q}^T(s) \right] (\underline{\theta}^* - \underline{\theta}) = \sum_{\Omega_I} \underline{q}(s) e(s) \quad (2)$$

Since  $E(\underline{q}(s)e(s)) = 0$  by (2.2) and  $\left[ \sum \underline{q}(s) \underline{q}^T(s) \right]$  is a positive definite matrix, the consistency of the estimate  $\underline{\theta}^*$  follows.

[•]

ii) To make our calculations easy we assume from now on that  $e(s)$  is normally distributed. Multiplying (2) by its transpose and taking expectations, we have

$$\begin{aligned} E \left[ \sum_s \underline{q}(s) \underline{q}^T(s) (\underline{\theta}^* - \underline{\theta}) (\underline{\theta}^* - \underline{\theta})^T \left( \sum_s \underline{q}(s) \underline{q}^T(s) \right)^T \right] \\ = E \left[ \sum_s \underline{q}(s) e(s) \sum_r (\underline{q}(r) e(r))^T \right] \end{aligned} \quad (3)$$

$$= \sum_s \sum_r E(\underline{q}(s) e(s)) E(\underline{q}^T(r) e(r))$$

$$+ \sum_s \sum_r E(\underline{q}(s) e(r)) E(\underline{q}^T(r) e(s))$$

$$+ \sum_s \sum_r E(e(s)e(r)) E(q(r)q^T(s)) \quad (4)$$

$$= I + II + III, \text{ where} \quad (5)$$

$$I = 0, \quad \text{by using (2.2);} \quad (6)$$

$$II = 2 M^2 v^2 I_{mxm}, \text{ by using (2.2);} \quad (7)$$

$$III = v \sum_s E(q(s)q^T(s)) \\ - v \sum_r \sum_{\substack{s \\ (s-r) \in N}} \theta_{(s-r)} E(q(r)q^T(s)) \quad (8)$$

Defining

$$E(q(s)q^T(s)) = \underline{Q}, \quad \text{mxm matrix}$$

$$E(q(r)q^T(s)) = \underline{T}_{r,s}, \quad \text{mxm matrix}$$

$$III = M^2 v \underline{Q} - v \sum_s \sum_{\substack{r \\ (s-r) \in N}} \theta_{(s-r)} \underline{T}_{r,s} \quad (9)$$

Substituting (6), (7), and (9), we see that

RHS of (3)

$$= M^2 [v \underline{Q} + 2v^2 I_{mxm} - v \sum_s \sum_{\substack{r \\ (s-r) \in N}} \theta_{(s-r)} \underline{T}_{r,s}] \quad (10)$$

for large values of  $M$

$$\frac{1}{M^2} \sum_s \underline{q}(s) \underline{q}^T(s) = \underline{q} + \eta(M), \quad (11)$$

where  $\eta(M)$  is such that

$$E(\eta^2(M)) = O\left(\frac{1}{M^2}\right)$$

Using (11) we obtain

$$(\text{LHS of (3)})/M^4 =$$

$$E[(\underline{q} + \eta(M))(\underline{\theta}^* - \underline{\theta})(\underline{\theta}^* - \underline{\theta})^T(\underline{q} + \eta(M))^T] \quad (12)$$

$$= \underline{q} E(\underline{\theta}^* - \underline{\theta})(\underline{\theta}^* - \underline{\theta})^T \underline{q}^T + O(1/M^2), \quad (13)$$

Substitution of (10) and (13) into (3) yields

$$\begin{aligned} E(\underline{\theta}^* - \underline{\theta})(\underline{\theta}^* - \underline{\theta})^T &= \frac{1}{M^2} [v \underline{q}^{-1} + 2v^2(\underline{q}^2)^{-1} \\ &\quad - \frac{v}{M^2} \underline{q}^{-1} \sum_s \sum_r \theta_{(s-r)} \underline{T}_{r,s}(\underline{q})^{-1} + O(1/M^4)] \end{aligned} \quad (14)$$

Q.E.D.

c) For the isotropic conditional model with  $N_S = \{(0,1), (1,0)\}$ , (14) reduces to

$$E(\underline{\theta}^* - \underline{\theta})^2 = \frac{1}{M^2} \frac{1}{(E(q^2(s)))^2} [4v^2$$

$$+ vE(q^2(s)) - \theta v \sum_{\substack{s \\ (s-r) \in N}} \sum_r E(q(s)q(r))] \quad (15)$$

where

$$\begin{aligned} q(s) = & y(s+(0,1)) + y(s+(0,-1)) \\ & + y(s+(1,0)) + y(s+(-1,0)) \end{aligned} \quad (16)$$

Let

$$\gamma_{k,l} = E[y(s)y(s+(k,l))] \quad (17)$$

Note

$$\gamma_{k,l} = \gamma_{-k,-l} \text{ and } \gamma_{l,k} = \gamma_{k,l} \quad (18)$$

Express the higher order correlations  $\gamma_{2,1}$ ,  $\gamma_{1,-2}$ ,  $\gamma_{2,0}$  and  $\gamma_{3,0}$  in terms of  $\gamma_{0,0}$ ,  $\gamma_{0,1}$ ,  $\gamma_{1,0}$  and  $\gamma_{1,1}$  by

$$\gamma_{0,0} = v/(1-4\theta\alpha_{1,0}) \quad (19)$$

$$\gamma_{2,1} = \frac{1}{2\theta} \gamma_{1,1} - \gamma_{1,0} \quad (20)$$

$$\gamma_{3,0} = \gamma_{1,0} \left\{ 1 + \frac{1}{\theta^2} \right\} - \frac{\gamma_{0,0}}{\theta} - \frac{3\gamma_{1,1}}{2\theta} - \frac{3\gamma_{1,-1}}{2\theta} \quad (21)$$

$$\gamma_{2,0} = \frac{1}{\theta} \gamma_{1,0} - \gamma_{1,-1} - \gamma_{0,0} - \gamma_{1,1} \quad (22)$$

$$\gamma_{1,-2} = \frac{1}{2\theta} \gamma_{1,-1} - \gamma_{1,0} \quad (23)$$

Equations (19-23) can be obtained by multiplying  $y(s)$  by appropriately shifted  $y(s+(k,l))$  and taking expectations.

Consider the various terms in (15).

$$E(q^2(s)) = \frac{1}{\theta} 4\gamma_{1,0} \quad (24)$$

$$\begin{aligned} \sum_s \sum_r \substack{(s-r) \in N} E(q(s)q(r)) &= 4[\theta \gamma_{1,0} + \gamma_{3,0} + 3\gamma_{2,1} + 3\gamma_{1,-2}] \\ &= 4[4\gamma_{1,0} + \frac{1}{2} \gamma_{1,0} - \frac{1}{\theta} \gamma_{0,0}] \end{aligned} \quad (25)$$

Substitution of (24) and (25) in (15) yields

$$E(\theta^* - \theta)^2 = \frac{1}{M^2} \frac{\theta^2}{16\gamma_{1,0}^2} [4v^2 + 4v\gamma_{0,0} - 16\theta\gamma_{1,0}v]$$

which on using (19) and  $\alpha_{1,0} = \gamma_{1,0}/\gamma_{1,1}$  gives

$$E(\theta^* - \theta)^2 = \frac{2\theta^2(1-4\theta\alpha_{1,0})^2}{4M^2\alpha_{1,0}^2}$$

Table 1.\* Computation of Asymptotic Variances and Efficiencies  
of Different Estimates in Isotropic Conditional  
Model with  $N_S = \{(0,1), (1,0)\}$

$\theta_0$	$M^2 \text{var}(\hat{\theta}_{ML})$	$M^2 \text{var}(\theta_C)$	$M^2 \text{var}(\theta^*)$	$\text{eff}(\theta_C)$	$\text{eff}(\theta^*)$
.1	.4928	.497	.494	.991	.9975
.2	.472	.489	.478	.965	.987
.3	.437	.474	.450	.921	.971
.4	.390	.454	.412	.859	.946
.5	.333	.427	.365	.779	.912
.6	.267	.393	.309	.681	.864
.7	.197	.349	.244	.564	.807
.8	.1243	.296	.1753	.419	.709
.9	.0556	.224	.1004	.248	.553

\*Column 5 is from [9].



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